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(54) Titre : NOUVELLES POLYUREES S'INSPIRANT DU DIISOCYANATE D'ISOPHORONE (DIIP), DU HEXAMETHYLENEDIISOCYANATE (HDI), LEURS ISOCYANURATES ET AMINES

(54) Title: NOVEL POLYUREAS BASED ON IPDI, HDI, THEIR ISOCYANURATES AND AMINES

(57) Abrégé/Abstract:
Disclosed is a novel polyurea based on (A) an isocyanate compound that is isophorone diisocyanate (IPDI), hexamethylene diisocyanate (HDI) or their isocyanurate and (B) a diamine or polyamine, such as isophorone diamine (IPD). The polyurea remain stable in a solid form at a curing temperature of 150-220°C standard for powder coating without releasing a significant quantity of organic materials or water and is useful in the paint industry.

23443-741

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Novel Polyureas Based on IPDI, HDI, their Isocyanurates and Amines

The present invention relates to novel polyureas based on (A) isophorone diisocyanate (IPDI), hexamethylene diisocyanate (HDI) and/or their isocyanurate and (B) amines, in particular isophorone diamine (IPD).

Polyureas are well known and are applied in the following technical areas as adhesives: wood and paper, foamed materials and resins for paints and coatings (see, for example, Houben-Weyl E 20/2 (1987), pp. 1721-1751; Houben-Weyl XIV/2 (1963), pp. 165-171).

A major object of the invention is to develop novel polyureas which remain stable in solid form at curing temperatures of 150 to 20°C standard for powder coatings, without releasing significant quantities (≤ 2 wt %) of organic materials or water.

Thus, the present invention provides polyureas based on (A) isocyanate compounds selected from isophorone diisocyanate (IPDI), hexamethylene diisocyanate (HDI) and their isocyanurates and (B) amines, with an NCO/NH_2 ratio of 0.9 to 1.1 to 1 and an average molecular mass (or weight) of at least 5,000.

The novel polyureas are formed from (A) isocyanate compounds that are isophorone diisocyanate (IPDI) or hexamethylene diisocyanate (HDI) and (B) amines, in particular isophorone diamine (IPD) as starting compounds. The IPDI and/or HDI can be used either as diisocyanate or as isocyanurate. Mixtures of both these isocyanates or their isocyanurates are also of advantage and suitable here.

Any aliphatic, (cyclo)aliphatic, cycloaliphatic and aromatic diamines and/or polyamines, preferably those having 5 to 18 carbon atoms (e.g., 6 to 12 carbon atoms), particularly preferably isophorone diamine (IPD), can be used within the scope of the invention. The term "(cyclo)aliphatic diamine or polyamine" means a compound in which at least one amino group is attached to an aliphatic moiety and at least one amine group is attached to a cycloaliphatic moiety.

In general, polyureas with an NCO/NH_2 ratio of 0.9 to 1.1 to 1 are manufactured. Solid and brittle polymers with a maximum degree of crosslinking, which melt only above 240°C with decomposition and are insoluble in solvents, are obtained with the addition of equimolar quantities having an NCO/NH_2 ratio of 1 to 1. Such polyureas generally have an average molecular weight of at least 5,000. The maximum is not critical. Often the polyureas have the average molecular weight not more than 50,000.

Preferred polyureas within the scope of the present invention are those comprising IPD and IPDI isocyanurate and/or HDI isocyanurate and mixtures thereof. As is well known, the isocyanurate is a trimer of the diisocyanate (i.e., IPDI or HDI) and has three isocyanate groups in addition to an isocyanurate ring. Often, the isocyanurate also contains a higher polymer as byproducts.

Another aspect of the present invention provides a process for manufacturing the polyureas, wherein the amine is employed in an inert solvent (preferably a hydrocarbon solvent such as toluol), to which the isocyanate, also diluted with a solvent, if required, is added with stirring. For complete conversion, the reaction mixture is heated for 2 to 3 hours with reflux of the solvent, is then cooled, the resulting

polymer is separated off (filtration) and then dried for 3 to 6 hours at 130 to 170°C in a vacuum.

The polyureas according to the present invention can be used as raw materials in the paint industry, in particular for manufacturing lacquers, paints and coatings.

The invention will now be described in greater detail by the following examples.

Examples

General manufacturing process

70 g IPD, diluted in 1000 ml toluol, are placed in a 2-liter triple-necked flask fitted with stirrer, drip funnel and heating mantle. The equivalent (NH_2 : NCO = 1:1) quantity of the corresponding isocyanate or a mixture, diluted with the same quantity of toluol, is then gradually added dropwise to the amine solution. After such addition, the reaction mixture is heated for 2 hours under reflux. After cooling to ambient temperature the corresponding solid (polyurea) is then filtered off and dried in a vacuum (3 to 6 hours at 130 to 170°C).

Polyurea examples (Data in mass parts)

	IPD	IPDI	IPDI trimer[1)]	HDI trimer[2)]
PH-1	70	-	183	-
PH-2	70	-	-	138
PH-3	70	61	61	-
PH-4	70	-	91	69

*Trade-mark

[1)]VESTANAT* T 1890, Degussa-Hüls AG

[2)]DESMODUR* N 330, Bayer AG

All products are white/colorless, brittle solids which are insoluble in standard solvents and melt only above 240°C with decomposition.

When using the above-described polyureas in powder coatings, for example, it is an advantage to grind the products into powder and screen them out to ≤ 100 µm.

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CLAIMS:

1. A polyurea based on:

(A) at least one isocyanate compound selected from the group consisting of isophorone diisocyanate (IPDI), an isocyanurate thereof, hexamethylene diisocyanate (HDI) and an isocyanurate thereof; and

(B) a diamine or polyamine with an NCO/NH_2 ratio of 0.9 to 1.1 to 1 and an average molecular mass of at least 5,000.

2. The polyurea as claimed in claim 1, wherein the isocyanate compound (A) is isophorone diisocyanate (IPDI) and the diamine or polyamine (B) is isophorone diamine (IPD).

3. The polyurea as claimed in claim 1, wherein the isocyanate compound (A) is the isocyanurate of isophorone dissocyanate (IPDI) and the diamine or polyamine (B) is, isophorone diamine (IPD).

4. The polyurea as claimed in claim 1, wherein the isocyanate compound (A) is a mixture of isophorone diisocyanate (IPDI) and IPDI isocyanurate and the diamine or polyamine (B) is isophorone diamine (IPD).

5. The polyurea as claimed in claim 1, wherein the isocyanate compound (A) is hexamethylene diisocyanate (HDI) and the diamine or polyamine (B) is isophorone diamine (IPD).

6. The polyurea as claimed in claim 1, wherein the isocyanate compound (A) is the isocyanurate of hexamethylene diisocyanate (HDI) and the diamine or polyamine (B) is isophorone diamine (IPD).

7. The polyurea as claimed in claim 1, wherein the isocyanate compound (A) is a mixture of hexamethylene diisocyanate (HDI) and HDI isocyanurate and the diamine or polyamine (B) is isophorone diamine (IPD).

8. The polyurea as claimed in claim 1, wherein the isocyanate compound (A) is a mixture of isophorone diisocyanate (IPDI) isocyanurate and hexamethylene diisocyanate (HDI) isocyanurate and the diamine or polyamine (B) is isophorone diamine (IPD).

9. The polyurea as claimed in any one of claims 1 to 8, which is solid at room temperature and is insoluble in solvents.

10. A polyurea based on:

(A) at least one isocyanate compound selected from the group consisting of isophorone diisocyanate (IPDI), an isocyanurate trimer thereof, hexamethylene diisocyanate (HDI) and an isocyanurate trimer thereof, and

(B) an aliphatic, (cyclo)aliphatic, cycloaliphatic or aromatic diamine having 5 to 18 carbon atoms,

with an NCO/NH_2 ratio of from 0.9:1 to 1.1:1 and an average molecular mass of at least 5,000,

wherein the polyurea is solid at room temperature and remains stable in the solid form at a temperature from 150°C to 220°C without releasing 2% by weight or more of organic materials or water.

11. The polyurea as claimed in claim 10, which is in a ground powder form adapted for use in powder coating.

12. The polyurea as claimed in claim 10 or 11, wherein the diamine (B) is a (cyclo)aliphatic diamine having 6 to 12 carbon atoms.

13. A process for manufacturing the polyurea as claimed in any one of claims 1 to 12, which comprises:

adding the isocyanate compound to the diamine or polyamine in a solvent, with stirring;

heating the resulting mixture for 2 to 3 hours with reflux of the solvent to from the polyurea;

cooling the resulting polyurea;

separating off the polyurea from the solvent; and

then drying the polyurea for 3 to 6 hours at 130 to 170°C in a vacuum.

14. Use of the polyurea as claimed in any one of claims 1 to 9, as a raw material in a paint industry.

15. Use of the polyurea as claimed in any one of claims 1 to 9, for manufacturing a lacquer, paint or coating.

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